

Low-lying excitations around a single vortex in a d-wave superconductor

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A full quantum-mechanical treatment of the Bogoliubov-de Gennes equation for a single vortex in a d-wave superconductor is presented. First, we find low-energy states extended in four diagonal directions, which have no counterpart in a vortex of s-wave superconductors. The four-fold symmetry is due to '*quantum effect*', which is enhanced when $p_F\xi$ is small. Second, for $p_F\xi \sim 1$, a peak with a *large energy gap* $E_0 \sim \Delta$ is found in the density of states, which is due to the formation of the lowest bound states.

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After a few years of controversy, d-wave nature of the high- T_c superconductors is now well established [1, 2], although superconductivity in the electron-doped $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ appears to be of s-wave [3]. Therefore it is important to understand the nature of vortex states in a d-wave superconductor [2, 4]. An earlier analysis of the vortex state based on the Gor'kov equation shows that a square lattice of vortices tilted by $\pi/4$ from the a-axis is the most stable except in the immediate vicinity of $T = T_c$ or in a weak magnetic field [5]. Such a square lattice of vortices, though distorted, has been seen by a small angle neutron scattering [6] and a scanning tunneling microscopy (STM) [7] in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ (YBCO) at low temperatures ($T < 10\text{K}$). We believe that this distortion of the vortex lattice is due to the orthorhombicity of the YBCO, although there are alternative interpretations based on the (d+s) admixture [8, 9]. One of the most remarkable results in the STM experiment is that the vortex appears to have a circular symmetry as in an s-wave superconductor. It is in sharp contrast to earlier results obtained within the Eilenberger theory (a semi-classical theory of a superconductor) [10], where a clear four-fold symmetry was obtained in the local density of states [11, 12, 13]. Further, at the center of the vortex, a peak with a *large energy gap* $E_0 \sim \Delta$ was found in the local density of states, where Δ is the superconducting order parameter. Then the most natural interpretation is that this corresponds to the lowest bound state for a vortex in a d-wave superconductor analogous to the one predicted by Caroli, de Gennes and Matricon [14].

In the previous study [15], in order to understand the results from the STM experiment, we have solved the Bogoliubov-de Gennes (B-dG) equation for a d-wave superconductor and obtained quasi-particle spectra around a single vortex. In the temperature region where the Ginzburg-Landau (GL) theory is valid, we found that the local density of states exhibits a circular symmetry and a peak with a *large energy gap* $E_0 \sim \Delta$ is found in the local density of states at the center of the vortex, which is consistent with the STM experiment. In ref. [15], it is crucial to set $p_F\xi \sim 1$ for YBCO, where p_F and ξ are the Fermi momentum and the coherence length respectively. The value of $p_F\xi$ is obtained by an approximate formula for the lowest bound state $E_0 = \Delta/(\pi p_F\xi)$ [12, 16]. This is also consistent with the chemical potential of YBCO deduced from the analysis of the spin gap seen in an inelastic neutron scattering experiment from monocrystals of YBCO [17, 18]. In the above analysis, however, we neglected the *noncommutability between \hat{k} and \mathbf{x}* ('*quantum effect*')[19], where \hat{k} and \mathbf{x} are the quasi-particle momentum and coordinate respectively, and the local density of states has a *perfect* circular symmetry except when the mixing of an s-wave component occurs [20]. The correction is $O(1/p_F\xi)$ and irrelevant at least in the study of systems with a long coherence length *e.g.* the superconducting phases of the heavy-fermion systems ($p_F\xi \sim 10$) and the ^3He superfluidity ($p_F\xi \sim 100$), but may have a serious influence in the study of the high- T_c superconductors, where $p_F\xi \sim 1$ as is discussed above.

In this paper, a full quantum-mechanical treatment of the B-dG equation for a d-wave superconductor is reported, where the '*quantum effect*' is taken into account. As shown below, the four-fold symmetry appears in the local density of states. Similar four-fold

symmetry was obtained in the previous studies [11, 12, 13]. But it should be noted that the four-fold symmetry discussed here has totally different origin from that obtained in the earlier studies. The B-dG equation for a d-wave superconductor is given by

$$\begin{aligned} & \left\{ -\frac{1}{2m}(\nabla - ie\mathbf{A}(\mathbf{x}))^2 - \mu \right\} u_n(\mathbf{x}) \\ & - \{ \partial_x(\Delta(\mathbf{x})\partial_x) - \partial_y(\Delta(\mathbf{x})\partial_y) \} v_n(\mathbf{x}) = \epsilon_n u_n(\mathbf{x}), \\ & - \left\{ -\frac{1}{2m}(\nabla + ie\mathbf{A}(\mathbf{x}))^2 - \mu \right\} v_n(\mathbf{x}) \\ & - \{ \partial_x(\Delta(\mathbf{x})^*\partial_x) - \partial_y(\Delta(\mathbf{x})^*\partial_y) \} u_n(\mathbf{x}) = \epsilon_n v_n(\mathbf{x}), \end{aligned}$$

where $u_n(\mathbf{x})$ and $v_n(\mathbf{x})$ are the quasi-particle amplitudes, $\Delta(\mathbf{x})$ is the pair potential, $\mathbf{A}(\mathbf{x})$ is the vector potential which is neglected assuming $H \ll H_{c2}$, and μ is the chemical potential which is identified with the Fermi energy. The parameters are set as $2m\xi^2\Delta = 2.82$ and $R/\xi = 30$, where ξ is the coherence length and R is radius of the system and the pair potential $\Delta(\mathbf{x})$ is given by

$$\Delta(\mathbf{x}) = \Delta \tanh(r/\xi) e^{i\phi}, \quad (0.1)$$

where r and ϕ are defined by $\mathbf{x} = (r \cos(\phi), r \sin(\phi))$. This form of pair potential is obtained by the Ginzburg-Landau (GL) theory for a d-wave superconductor [12, 20] and applicable at not too low temperatures (an estimate of the temperature region where the GL theory is valid is $[0.5T_c, T_c]$ for an s-wave superconductor, when one consider the quasi-particle spectra around a single vortex).

In order to solve the B-dG equation numerically, it is convenient to expand the quasi-particle amplitudes $u_n(\mathbf{x})$ and $v_n(\mathbf{x})$ as

$$\begin{aligned} u_n(\mathbf{x}) &= \sum_{l=-\infty}^{\infty} \sum_{j=1}^{\infty} u_{n,l,j} \psi_{j,|l|}(r) \exp(il\phi), \\ v_n(\hat{k}) &= \sum_{l=-\infty}^{\infty} \sum_{j=1}^{\infty} v_{n,l,j} \psi_{j,|l-1|}(r) \exp(i(l-1)\phi). \end{aligned}$$

Here $\psi_{i,\nu}(x) = \frac{1}{\sqrt{2\pi R J_{\nu+1}(\alpha_{i,\nu})}} J_{\nu}(\alpha_{i,\nu} x/R)$ ($J_{\nu}(x)$ is the Bessel function), $\alpha_{j,\nu}$ is the j -th positive zero point of $J_{\nu}(x)$ and R is the radius of the system. In the previous study [15], in which the 'quantum effect' is neglected, the B-dG equation decouples for $u_{n,l,j}$'s and $v_{n,l,j}$'s with different l . On the other hand, when the 'quantum effect' is taken into account, $u_{n,l,j}$'s and $v_{n,l,j}$'s with different l couple, which plays an important role when $p_F\xi$ is small. Because of the coupling, the number of basis we can use for numerical diagonalization is small compared to the previous study [15]. However, it is sufficient for the understanding of the qualitative aspects.

At first, consider the density of states $\sum_i \delta(E - E_i)$ as a function of E/Δ , where $p_F\xi = 1.33$. As is seen in Fig. 1, there is a peak with a *large energy gap* $E_0 \sim \Delta$. This

corresponds to the lowest bound state. The peak has a width due to the internal degree of freedom in the \hat{k} space. These are consistent with the previous results [15] qualitatively, where the '*quantum effect*' is neglected.

Next consider a local density of states in a superconductor, which is the quantity of interest for comparison to STM experiments and given by,

$$N(E, \mathbf{x}) = \sum_n [|u_n(\mathbf{x})|^2 \delta(E - \epsilon_n) + |v_n(\mathbf{x})|^2 \delta(E + \epsilon_n)].$$

In Fig. 2 and 3, $\int_0^{0.35\Delta} dE N(E, r, \phi)$ is plotted and they show a clear four-fold symmetry in the local density of states. When $p_F \xi$ is changed from 1.33 to 2.00, the four-fold symmetry is suppressed (see Fig. 3) and the local density of states becomes circular. This supports the idea that the four-fold symmetry is due to the '*quantum effect*'. We stress that these low-energy states extended in four diagonal directions are particular to d-wave superconductivity. Therefore 1) these states should give rise to the zero-energy density of states proportional to \sqrt{B} as discussed by Volovik and others [21, 4], 2) they are the most likely the origin of the large flux flow resistivity in YBCO observed recently by Doettinger et al. [22] and, 3) when a square lattice of vortices tilted by $\pi/4$ from the a-axis is formed, the quasi-particle can move from one vortex to the other through these low-energy states extended in four diagonal directions, which should give rise to a cohesive energy guaranteeing the stability of the square lattice. The clarification of the quasi-particle spectrum in a vortex lattice and, in particular, the tilted square lattice is of immediate interest.

In conclusion, we have investigated the Bogoliubov-de Gennes equation for a d-wave superconductor, where the *noncommutability between \hat{k} and \mathbf{x}* ('*quantum effect*') is taken into account. We found a peak with a *large energy gap* $E_0 \sim \Delta$ in the density of states, which is consistent with the previous results. We found low-energy states extended in four diagonal directions, which is due to the '*quantum effect*'. The low-energy states have no counterpart in a vortex of s-wave superconductors. It is natural to consider that these low-energy states cause directional attractive forces between vortices. It is possible that, due to the directional attractive force, a square lattice of vortices becomes stable in some parameter region. Another scenario for a square lattice of vortices is proposed in ref. [5], where the higher-order correction in the Ginzburg-Landau theory [23] plays an essential role. In this paper, we do not consider the effect of the higher-order correction. The higher-order correction causes the four-fold symmetry in the pair potential. We consider that, in low temperatures, it is needed to take into account both the '*quantum effect*' and the higher-order correction in the GL theory self-consistently, and more detailed study is left as a future problem.

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Figure Captions

Fig. 1: $\sum_i \delta(E - E_i)$ as a function of E/Δ , where $k_F\xi = 1.33$.

Fig. 2: $\int_0^{0.35\Delta} dE N(E, r, \phi)$, where $k_F\xi = 1.33$ for a) $r/\xi = 3.0$, b) $r/\xi = 9.0$, c) $r/\xi = 15.0$ and d) $r/\xi = 27.0$.

Fig. 3: $\int_0^{0.35\Delta} dE N(E, r, \phi)$, where a) $k_F\xi = 1.33$ and $r/\xi = 9.0$ and b) $k_F\xi = 2.0$ and $r/\xi = 9.0$.

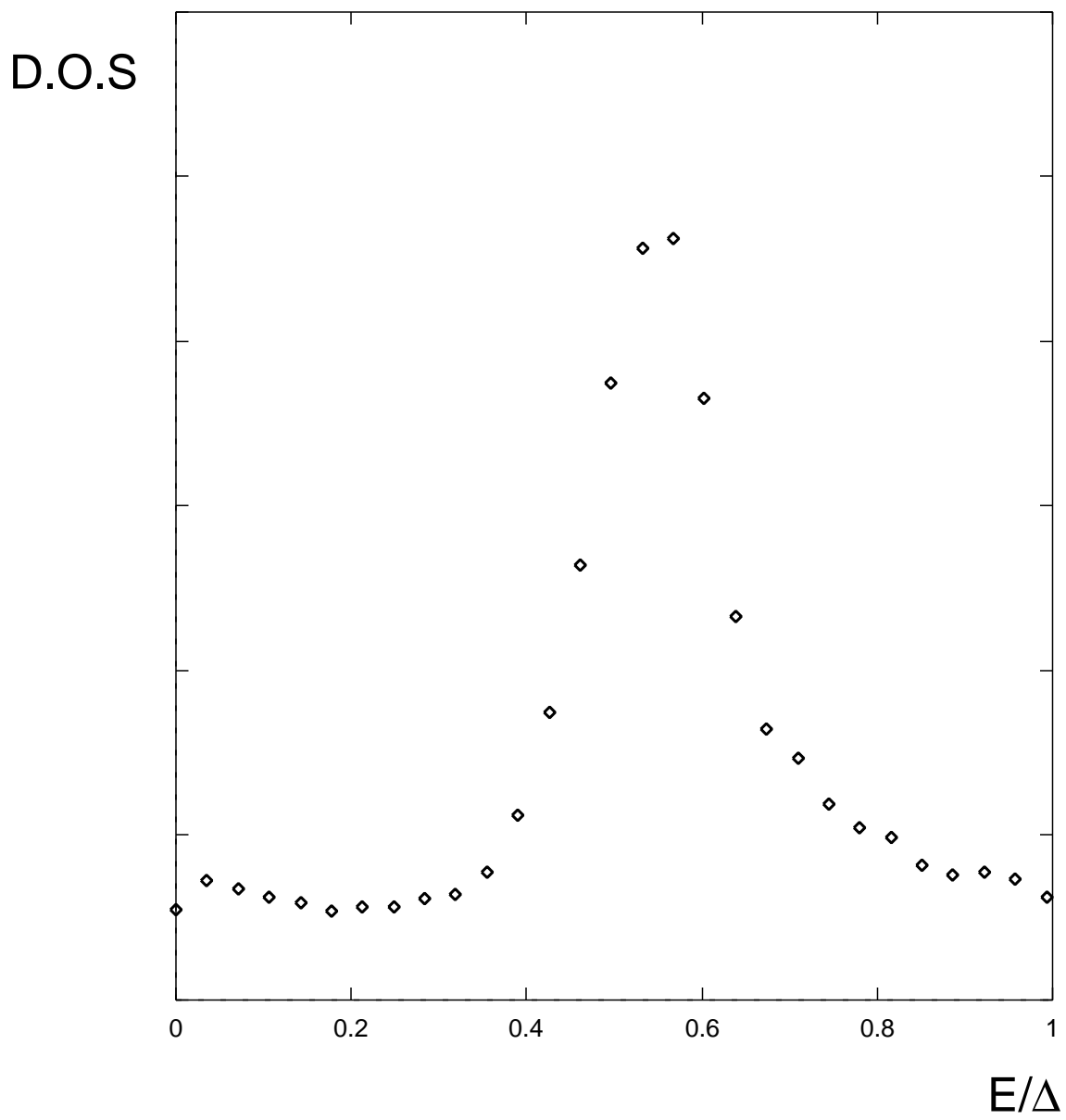


Fig. 1

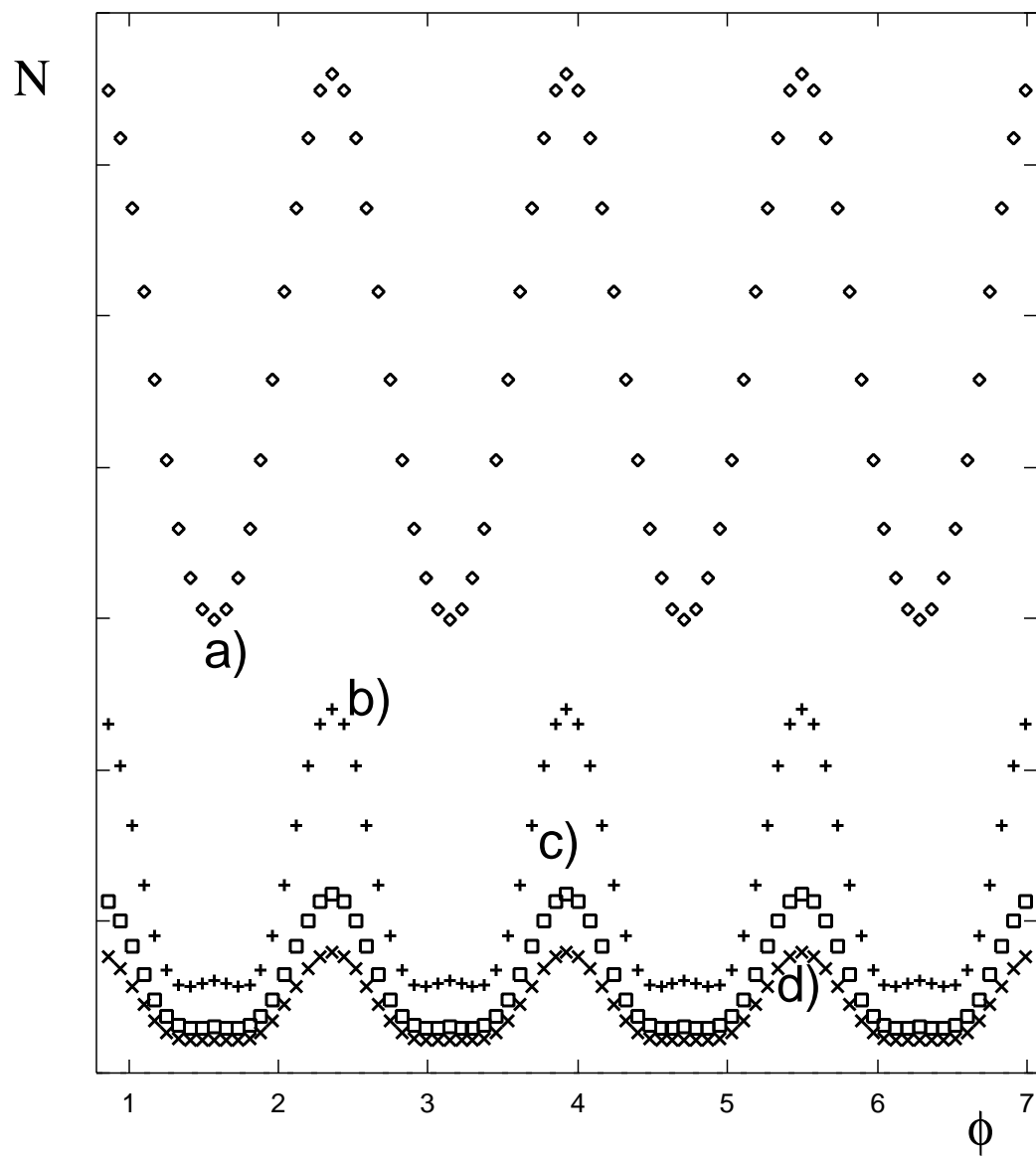


Fig. 2

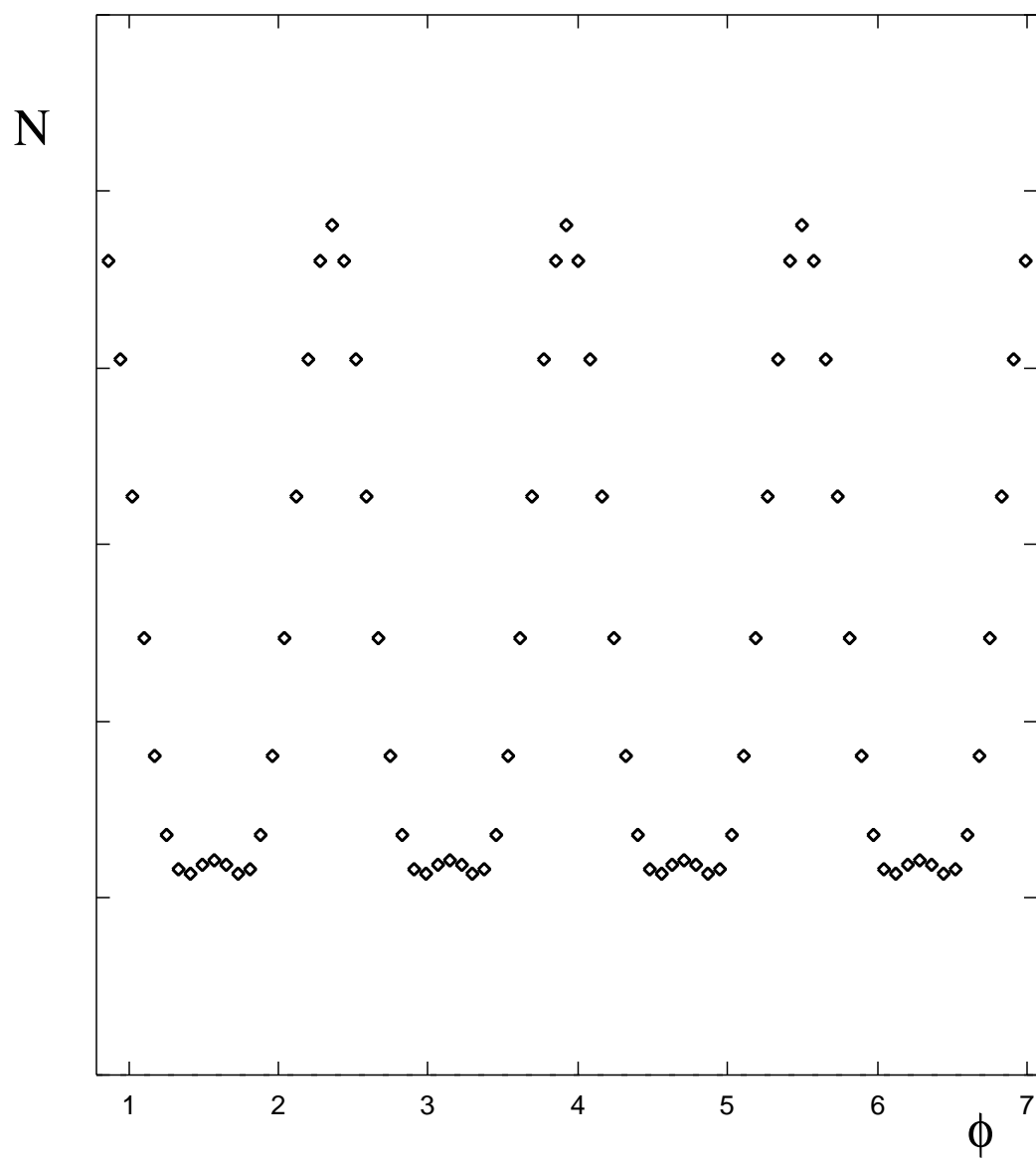


Fig. 3 a)

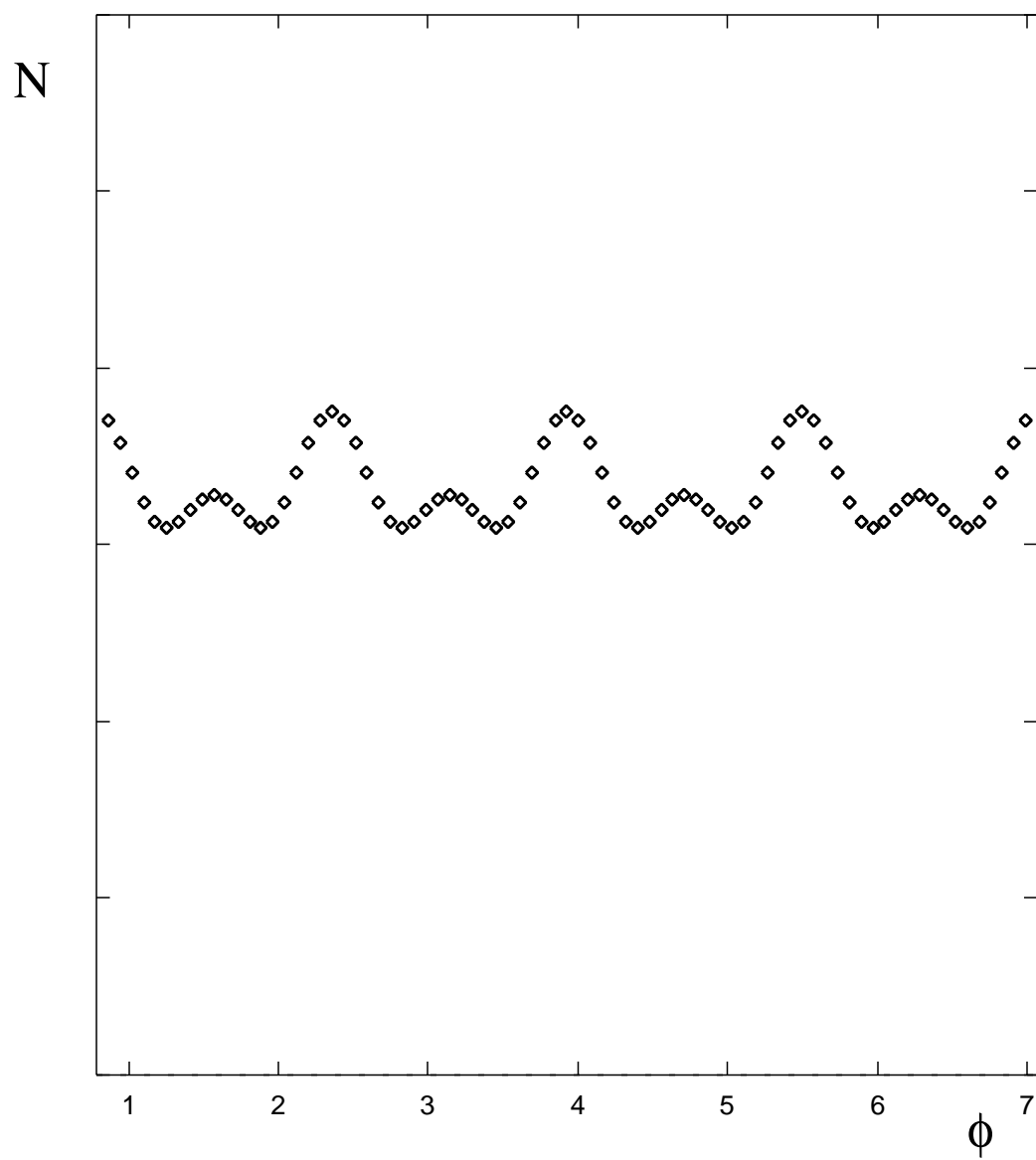


Fig. 3 b)